

Adiabatic demagnetization and generation of entanglement in spin systems

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Abstract

We study the entanglement emergence in a dipolar-coupled nuclear spin-1/2 system cooled using the adiabatic demagnetization technique. The unexpected behavior of entanglement for the next- and next-next-neighbor spins is revealed: entangled states of a spin system appear in two distinct temperature and magnetic field regions separated by a zero-concurrence area. The magnetic field dependence of the concurrence can have two maximums which positions are determined by the initial conditions and number of spins in a chain.

I. INTRODUCTION

Prospects for practical application of quantum technology and devices based on entangled state stimulate intensive qualitative and quantitative research of quantum entanglement in various physical systems. Among these systems, a system of nuclear spins presents excellent theoretical and experimental models for studying the entanglement properties. Systems with a large number of spins with various models of the spin interaction have been described in a number of papers, see e.g. [1–5], and the references therein. However, a major part of the performed studies considers the temperature and field dependences without taking into consideration the realistic cooling technique for achieving low temperature at which entanglement appears. Adiabatic demagnetization (AD) performed by variations of an external magnetic field is a very useful and effective technique for the attainment of proper low temperatures, of the order of microkelvins, at which entanglement appears in spin systems [6–11].

Recently, using adiabatic demagnetization in the rotating frame (ADRF) [12–14], entanglement in a dipolar-coupled nuclear spin system was studied [15]. In contrast to the conventional AD method, ADRF uses an external magnetic field which is much stronger than internal dipolar field and a radiofrequency field with an offset from the Larmor frequency.

It was shown that there is no entanglement between remote spins, although the considered model included dipole interactions between these spins which is the typical condition to create entangled states.

In this paper we consider the entanglement emergence in a one-dimensional dipolar-coupled nuclear spin-1/2 system cooled using the conventional AD technique. We consider the case where the Zeeman energy is of the order of or even less than the dipolar interaction one.

The structure of the paper is as follows: in the next section, we describe the Hamiltonian for a spin system in an external field, conditions of the AD realization and analyze variations of the spin temperature T and magnetization M at AD. Then we consider the pairwise entanglement. Discussion of the results is given in the final section. The numerical calculation of the spin temperature, magnetization, heat capacity and concurrence C_{mn} between the m -th and n -th spins at arbitrary orientation of the magnetic field is performed using the software based on the MatLab package which allows us to consider systems of up to ten

spins.

A. Spin system at adiabatic demagnetization

We consider a linear system of N dipole-coupling nuclear spins $I = 1/2$ in an external magnetic field when the Zeeman energy of the order of or even less than the dipolar interaction one. The Hamiltonian of the system can be presented in the following form

$$H = H_z + H_{dd} \quad (1)$$

where the Hamiltonian H_z describes the Zeeman interaction between the nuclear spins and external magnetic field

$$H_z = \omega_0 \sum_{k=1}^N I_k^z, \quad (2)$$

$\omega_0 = \gamma |\vec{H}_0|$ is the energy difference between the excited and ground states of an isolated spin, \vec{H}_0 is the external magnetic field, γ is the gyromagnetic ratio of a spin, I_k^z is the projection of the angular spin momentum operator on the z - axes. The Hamiltonian H_{dd} describing dipolar interactions in an external magnetic field [14]:

$$H_{dd} = \sum_{j < k} \frac{\gamma^2}{r_{jk}^3} \left\{ (1 - 3 \cos^2 \theta_{jk}) \left[I_j^z I_k^z - \frac{1}{4} (I_j^+ I_k^- + I_j^- I_k^+) \right] - \frac{3}{4} \sin 2\theta_{jk} [e^{-i\varphi_{jk}} (I_j^z I_k^+ + I_j^+ I_k^z) + e^{i\varphi_{jk}} (I_j^z I_k^- + I_j^- I_k^z)] - \frac{3}{4} \sin^2 \theta_{jk} [e^{-2i\varphi_{jk}} I_j^+ I_k^+ + e^{2i\varphi_{jk}} I_j^- I_k^-] \right\} \quad (3)$$

where r_{jk} , θ_{jk} , and φ_{jk} are the spherical coordinates of the vector \vec{r}_{jk} connecting the j -th and k -th nuclei in a coordinate system with the z -axis along the external magnetic field, \vec{H}_0 , I_j^+ and I_j^- are the raising and lowering spin angular momentum operators of the j -th spin. We consider the case when $\omega_0 \sim D_{12} = \frac{\gamma^2}{r_{12}^3}$ (here D_{12} is the dipolar coupling constant for the nearest spins), and it is necessary to take into account all the terms of the Hamiltonian, and not truncate any ones.

Let us analyze conditions of the adiabatic demagnetization in the spin system. To prevent heat exchange between a spin system and a lattice, the evolution time of the considered spin system has to be much shorter than the spin-lattice relaxation time, T_1 . On the other hand,

decoherence in a spin system refers to how the system loses the quantum coherence features and can be characterized by time of the order of T_2 , the lifetime of the free precession signal ($T_2 \ll T_1$ [11, 13]). Decoherence times, $T_2 \sim (\gamma H_{loc})^{-1}$ (H_{loc} is the local magnetic field created by spins) for spin systems at low temperature typically range between nanoseconds and seconds [16]. In contrast to T_2 , T_1 takes values in the range from minutes to hours [11, 13]. For example, it was found in LiF at $T = 2\text{K}$ that $T_1 = 50$ min for ^{19}F and $T_1 = 15$ hours for Li [9]. If to choose the characteristic time of variation of the external field such that $t_{ch} > T_2$, the system can be considered as being in thermal equilibrium at every point of time and its density matrix is

$$\rho = \frac{1}{Z} \exp \left\{ -\frac{\beta H}{D_{12}} \right\}. \quad (4)$$

where β is the inverse spin temperature in units of D_{12} , $\beta = \frac{D_{12}}{k_B T}$, T is the spin temperature and $Z = \text{Tr} \left\{ \exp \left(-\frac{\beta H}{D_{12}} \right) \right\}$ is the partition function that encodes the statistical properties of a system in thermodynamic equilibrium.

A spin system can be considered in the thermal equilibrium during evolution if [9]

$$\frac{dH_0}{dt} \ll \gamma H_{loc}^2. \quad (5)$$

The mean local magnetic field H_{loc} determines by the following expression $H_{loc} = \frac{1}{\gamma} \sqrt{\frac{\text{Tr}(H_{dd}^2)}{\text{Tr} I_z^2}}$ and depends on the number of spins in the system [9]. Our calculations of this field for all cases considered below, $N = 2 \div 10$, give $H_{loc} = (0.8 \div 1.2) D_{12}$, where $D_{12} \sim 10$ G [9], which leads to the value of the order of few gauss. For example, in LiF calculation gives $H_{loc} = 7.77$ G [9]. With this value and $\gamma = 2\pi \times 4005.5 \frac{\text{Hz}}{\text{G}}$ Eq (5) gives that $\frac{dH_0}{dt} \ll 1.5 \times 10^6 \frac{\text{G}}{\text{s}}$. If we take $\frac{dH_0}{dt} = 1.5 \times 10^5 \frac{\text{G}}{\text{s}}$ the field change time from 6000 G to 10 G equals $t_{ch} = 4 \times 10^{-2}$ s that satisfies the condition of adiabaticity $T_1 \gg t_{ch} \geq T_2 \sim 10^{-5}$ s.

Thermodynamic variables of the system, such as entropy, S and heat capacity C , can be expressed in terms of the partition function or its derivatives. For example, the entropy S and heat capacity C are given by

$$S = k_B \frac{\partial (\beta \ln Z)}{\partial \beta} \quad (6)$$

and

$$C = k_B \beta^2 \frac{\partial^2 \ln Z}{\partial \beta^2}, \quad (7)$$

respectively. The magnetization M of the spin system can be also expressed in the terms of the partition function

$$M = -\frac{1}{\beta Z} \frac{\partial Z}{\partial B} \quad (8)$$

where B is the external magnetic flux density.

The variation of the parameters at AD is simulated by the following way. At an initial condition $\beta = \beta_{in}$ and $H_0 = H_{0in}$ the entropy is calculated using Eqs. (4) and (6), the external magnetic field is decreased and a new temperature is determined from the condition $S = const.$

Fig. 1 shows the inverse spin temperature versus the external magnetic field. One can see that the inverse spin temperature β is proportional to ω_0 at $\omega_0 \gg D_{12}$ for all the spin systems considered here. For $\omega_0 < D_{12}$ the inverse spin temperature is practically independent of ω_0 (see the inset of Fig.1). The main change of temperature occurs in the range of ω_0/D_{12} from 5 till 1. At $\omega_0/D_{12} > 5$ the inverse spin temperature increases approximately linearly with a decrease of the magnetic field. In contrast to the dependence of the temperature on the external magnetic field, the magnetization is about constant at $\omega_0 > 5D_{12}$ and decreases linearly with the magnetic field decrease at $\omega_0 < D_{12}$ (see the inset of Fig.2). At high fields $\omega_0 > 3D_{12}$, the temperature and magnetization became independent of the number of spins in the system.

In the region of high temperatures (low β), our results coincide with well-known dependencies obtained in the framework of the high temperature approximation $\left| \frac{\beta H}{D_{12}} \right| \ll 1$ for $N \gg 1$ (see dark yellow shot dash-dotted lines in Figs. 1 and 2) [9, 13]. We can see from Fig. 2 that the high temperature approximation is valid for $\omega_0 > D_{12}$ which corresponds to $\beta < 2.3$ (Fig.1). Below we will consider entanglement measures and temperature and field dependence of entanglement of the linear chain of dipolar coupled spins under AD.

B. Generation of entanglement at adiabatic demagnetization

There are several parameters characterizing the entangled state of a spin system: the von Neumann entropy, entanglement of formation, log negativity, concurrence of a pair of spins, and etc. [1, 2, 17–20]. We will characterize the entangled states by the concurrence between two, m -th and n -th, spins which is defined as [17]

$$C_{mn} = \max \{q_{mn}, 0\}, \quad (9)$$

with $q_{mn} = \lambda_{mn}^{(1)} - \lambda_{mn}^{(2)} - \lambda_{mn}^{(3)} - \lambda_{mn}^{(4)}$. Here $\lambda_{mn}^{(k)}$ ($k = 1, 2, 3, 4$) are the square roots of eigenvalues, in descending order, of the following non-Hermitian matrix:

$$R_{mn} = \rho_{mn} (\sigma_y \otimes \sigma_y) \tilde{\rho}_{mn} (\sigma_y \otimes \sigma_y), \quad (10)$$

where ρ_{mn} is the reduced density matrix. For the m -th and n -th spins, the reduced density matrix ρ_{mn} is defined as $\rho_{mn} = \text{Tr}_{mn}(\rho)$ where $\text{Tr}_{mn}(\dots)$ denotes the trace over the degrees of freedom for all spins except the m -th and n -th spins. In Eq. (10) $\tilde{\rho}_{mn}$ is the complex conjugation of the reduced density matrix ρ_{mn} and σ_y is the Pauli matrix $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. For maximally entangled states, the concurrence is $C_{mn} = 1$ while for separable states $C_{mn} = 0$. The concurrence for two-spin system in the thermal equilibrium is zero at $\theta = 0$ and $\theta = \pi$, and it reaches the maximum values at $\theta = \frac{\pi}{2}$ and $\varphi = 0$ [22]. We have confirmed these results by numerical calculations for all spin pairs in the chains with $N = 3, \dots, 10$. Therefore, we will restrict ourselves to the cases corresponding to the concurrence maximum.

Fig. 3 presents the results of numerical calculations of the concurrence and heat capacity as functions of the magnetic field at AD. With decreasing the magnetic field, the both quantities increase up to the maximum and then decrease till zero. Both, the concurrence and heat capacity decrease with increasing number of spins for and are practically independent of the spin number for .

Appearance of entanglement at AD and behavior of the concurrence depend on initial conditions: initial values of the magnetic field and temperature from which AD is started. This dependence is illustrated for a two-spin chain by the phase diagram of Fig. 4. If AD starts at point A (Fig.4) above the curve separating the entangled and separable states, a non-zero concurrence is observed till point a_1 where the AD phase trajectory crosses the boundary line (Figs. 4 and 5). Starting from point B we achieve the entangled state between points b_1 and b_2 , while starting from point C does not lead to appearance of the entangled state. The similar results are obtained for all neighboring spins in the chains with $N = 3, \dots, 10$.

The results for remote spins are presented in Figs. 6-8. At $\omega_0/D_{12} > 5.5$, the concurrence for the next-neighbor spins C_{13} has two maximums which are separated by area with zero

concurrence (Figs. 6 and 7). The zero concurrence area expands with increasing the spin number in a chain (Fig. 6) and the initial temperature (Fig. 7b) and reduces when the initial magnetic field increases (Fig. 7a). At AD the first maximum (at higher field) decreases with the increase of the spin number in a chain (Fig. 6) and of the initial magnetic field and temperature (Fig.7). The first maximum position moves towards higher magnetic fields with increasing spin number and initial temperature. The second maximum also moves towards higher magnetic fields with increasing the initial field (Fig. 6) but its position does not practically depend on the initial temperature (Fig.7).

The concurrence for next-next-neighbor spins C_{14} also has two maximums while only one maximum presents in the magnetic field dependence of the concurrence for the first and fifth spins C_{15} (Fig. 9). In all considered cases, the concurrency for remote spins practically does not depend on the number of spins for $N > 7$.

C. Discussion and conclusion

We have investigated entanglement in a linear chain of dipole-coupling spins $s = 1/2$ at AD which is one of the ways to achieve ultra-low spin temperatures.

The inverse temperature at which entanglement appears is $\beta \sim 2.3$. Let us estimate this temperature for fluorine in calcium-fluoride CaF_2 with the dipolar interaction energy of the order of a few kHz (in frequency units) [14]. Taking as in [14, 21] $H_0 = 3$ G we have $\omega_0 = 12$ kHz, which leads to $T = 0.34 \mu\text{K}$. The estimated value of temperature is in good agreement with those reported early for the spin system $s = 1/2$ with the XY Hamiltonian [4] and for the Hamiltonian of two dipolar coupling spins [22]. It is interesting that the transition to the ordered states, such as antiferromagnetic, of nuclear spins was observed in a single crystal of calcium-fluoride precisely at $T = 0.34\mu\text{K}$ [14, 21].

An unexpected behavior of the next nearest-neighbor and next-next nearest-neighbor concurrences was obtained: remote spins in the thermal equilibrium are entangled in two distinct temperature and magnetic field regions (Figs 6-8). In most studied cases the ground state at zero temperature is entangled [1, 2, 23]. However examples were found [20, 24] where the ground state is separable and there are two temperature regions of entangled states. We show that the same behavior takes place also for the field dependence of the concurrence (Fig.6) at certain initial values of the temperature and magnetic field (Fig. 4).

Our investigation demonstrates that the qualitative behavior of entanglement with temperature and magnetic field can be much more complicated than might otherwise have been expected. Thus, the AD technique allows one to generate entangled states between dipolar coupling spins in a linear chain. It opens a simple and effective way to the experimental testing of entanglement in spin systems.

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Figure captions

Fig. 1 Fig. 1 Inverse spins temperature as a function of applied field, ω , at AD in chains with various number of spins: black solid line - $N = 4$, red dashed line - $N = 5$, green dotted line - $N = 6$, blue dash-dotted line - $N = 7$, cyan dash-dot-dotted line - $N = 8$, magenta shot-dashed line - $N = 9$, yellow shot-dotted - $N = 10$, dark yellow shot-dash-dotted – the high temperature approximation for $N \gg 1$.

Fig. 2 Magnetization, as a function of applied field for an adiabatic demagnetization in chain with various number of spins: black solid line - $N = 4$, red dashed line - $N = 5$ green dotted line - $N = 6$, blue dash-dotted line - $N = 7$ cyan dash-dot-dotted line - $N = 8$, magenta shot-dashed line - $N = 9$, yellow shot-dotted $N = 10$, dark yellow shot-dash-dotted – the high temperature approximation for $N \gg 1$.

Fig.3 Field dependence of concurrence between the first and second spins (a) and of heat capacity C per spin (b) in various chains: black solid line - $N = 2$, red dashed line - $N = 3$, green dotted line - $N = 4$, blue dot-dashed line - $N = 5$, cyan dash-dot-dotted line - $N = 6$, magenta shot dashed line - $N = 7$, yellow shot dotted - $N = 8$, dark yellow shot dash-dotted - $N = 9$, navy - $N = 10$.

Fig. 4 The phase diagram for a two-spin system at AD started from various initial points: $A\{\omega_0 = 2.4, \beta = 1.06\}$; $B\{\omega_0 = 3, \beta = 0.7\}$; $C\{\omega_0 = 2.7, \beta = 0.443\}$. The black solid line is the boundary between the entangled and separable states; green dashed, red dotted, and blue dot-dashed lines show the phase trajectories started from A , B , C respectively.

Fig. 5 Field dependence of the concurrence at AD starting from initial conditions corresponding to $A\{\omega_0 = 2.4, \beta = 1.06\}$ (green dashed line) and $B\{\omega_0 = 3, \beta = 0.7\}$ (red dotted line) in the $\omega_0 - \beta$ diagram of Fig. 4.

Fig.6 Field dependence of concurrence for the first and third spins in various chains at AD starting from $\beta = 2$: black solid line - $N = 3$, red dashed line - $N = 4$ green dotted

line - $N = 5$, blue dash-dotted line - $N = 6$ cyan dash-dot-dotted line - $N = 7$, magenta shot-dashed line - $N = 8$, yellow shot-dotted line - $N = 9$, dark yellow shot-dash-dotted line - $N = 10$.

Fig.7 Field dependence of concurrence for the first and third C_{13} spins in 3-spin chain (a) and 6-spin chain (b) at AD starting from various initial points.

a) - initial inverse temperature $\beta = 1$ and various initial external magnetic fields: black solid line - $\omega_0/D_{12} = 5$; red dashed line - $\omega_0/D_{12} = 5.3$; green dotted line - $\omega_0/D_{12} = 5.5$; blue dash-dotted line - $\omega_0/D_{12} = 6$.

b)- initial external magnetic field $\omega_0/D_{12} = 20$ and various initial inverse temperatures: black solid line - $\beta = 0.3$; red dashed line - $\beta = 0.4$; green dotted line - $\beta = 0.6$; blue dash-dotted line - $\beta = 0.9$; cyan dash-dot-dotted line - $\beta = 1$; magenta shot-dashed line - $\beta = 3$.

Fig. 8 Field dependence of concurrence C_{14} for the first and fourth spins in various chains: (a) $N = 4$; (b) black solid line - $N = 5$, red dashed line - $N = 6$ green dotted line - $N = 7$ for the initial inverse temperature $\beta = 2$ and magnetic field $\omega_0/D_{12} = 40$.

Fig. 9 Field dependence of concurrence C_{15} for the first and fifth spins in various chains: black solid line - $N = 5$, red dashed line - $N = 6$, green dotted line - $N = 7$; for the initial inverse temperature $\beta = 2$ and magnetic field $\omega_0/D_{12} = 40$.

















